Scattering function of a ring polymer with fixed knot : An exact expression in the θ condition and that of the correlation function

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An exact expression in the θ condition and that of the correlation function

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We show an analytic expression for scattering function $g_K(q)$ of a ring polymer with fixed knot K in the theta condition. We discuss its asymptotic behavior, which suggests nontrivial topological entropic effects. We derive $g_K(q)$ via an empirical formula for the probability distribution of distance between two nodes in random polygon of knot K consistent with simulations.

シータ温度溶液中でトポロジー的拘束条件下にある環状高分子鎖の散乱関数と2点相関関数を表す解析的表式を数値シミュレーションの結果を援用して導出した。相関関数はある解析関数の積分の形に表される。散乱関数の高波数極限などは、数値的な取り扱いが微妙で困難である。しかし、この解析的方法により厳密に調べられる。その結果、興味深いクロスオーバーが示唆される。

1 Introduction and Conclusion

Ring polymers have attracted much interest in polymer physics, and their various properties have been studied not only theoretically but also experimentally such as using circular DNAs. [1] Recently ring polymers under topological constraints have been studied extensively. [2, 3] According to des Cloizeaux, a topological constraint should lead to an effective repulsion among segments of ring polymers, which has been numerically confirmed. [3]

Let us denote by $f(r; \lambda, N)$ the probability distributiuon of distance r between two nodes in a random polygon of N nodes having fixed knot type K. [4] For a given pair of nodes, say, j and k, out of the N nodes, we define parameter λ by the fraction n/N, if the two arcs between them have segments n and $N-n$ where $n \leq N-n$. Here $\boldsymbol{r}$ denotes the difference of the position vectors: $\boldsymbol{r} = \boldsymbol{R}_j - \boldsymbol{R}_k$, and $r = |\boldsymbol{r}|$. We propose the following formula for $f_K(r; \lambda, N)$:

$$f_K(r; \lambda, N) = C_K \, r^{2+\theta_K} \exp\left[\frac{-3r^2}{2N{\sigma_K}^2}\right] \tag{1}$$

where θ_K and σ_K are functions of variable $z = \lambda(1-\lambda)$ as

$$\sigma_K(z; N) = z^{\frac{1}{2}} \exp(\alpha_K \, z) \, , \quad \theta_K(z; N) = b_K z^{\beta_K} \, . \tag{2}$$

The parameters α_K, β_K and b_K depend on the knot K and the number of nodes, N.

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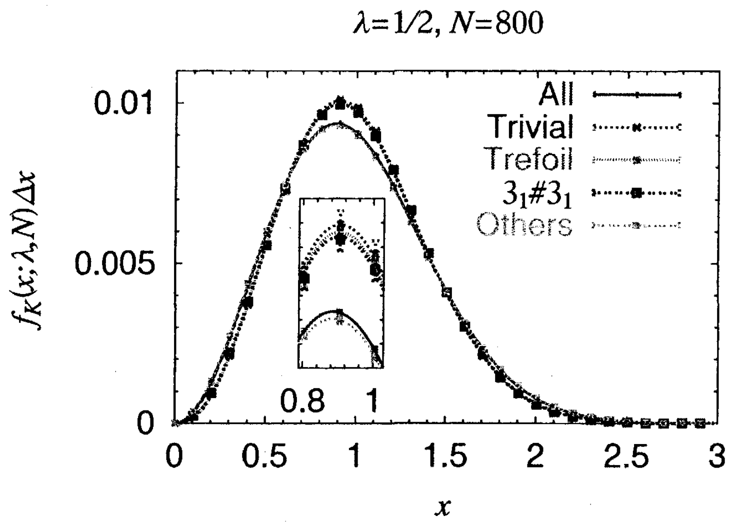

Figure 1: The normalized probability distribution $\tilde{f}_K(x;\lambda,N)$ for $\lambda=1/2$ and $N=800$, where $x=r/r_K$ for the average distance r_K. For knots, 0, 3_1, $3_1\#3_1$, *others* and *all*, θ_K are estimated by 0.454 ± 0.005, 0.413 ± 0.006, 0.389 ± 0.005, -0.033 ± 0.0005 and 0.002 ± 0.003, respectively. In the inset, the peaks are given by 0, 3_1, $3_1\#3_1$, *all* and *others*, respectively, in decreasing order.

The model function (1) of $f_K(r;\lambda,N)$ is consistent with simulation data as shown in Fig. 1. [6] The function (1) leads to an analytic expression of scattering function $g_K(q)$, which is consistent with that evaluated in recent simulation [5]. Moreover, for $q=|\vec{q}|\gg 1$ we have

$$\frac{g_K(q)}{N}=2\int_0^{1/2}\frac{\sqrt{2}\sin(\pi\theta_K(\lambda)+\pi/4)}{\Gamma(\{3+\theta_K(\lambda)\}/2)/(\sqrt{\pi}/2)}\left(\frac{Nq^2}{6}\sigma_K^2\right)^{\theta_K(\lambda)}\exp\left(-\frac{Nq^2}{6}\sigma_K^2\right)d\lambda+O(1/A) \quad (3)$$

where $A=Nq^2/12$ and we have a slow asymptotic expansion with $\beta_K\approx 0.5$:

$$\frac{g_K(q)}{N}=\frac{1}{A}\left(1+O(A^{-\beta_K})\right). \quad (4)$$

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